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ANALYTICAL REPRESENTATION OF ELASTIC SCATTERING CROSS SECTIONS OF LOW ENERGY ELECTRONS BY ATMOSPHERIC GASES

V.Ye. Ivanov, N.K. Osipov and V.A. Shneyder

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16. Abstract

Analytical representations of the elastic scattering cross sections of electrons with energies of 0.01-1 keV in atmospheric gases of N_2, O_2, O are given. These representations are suitable for the Monte Carlo method.

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ANALYTICAL REPRESENTATION OF ELASTIC SCATTERING CROSS SECTIONS OF LOW ENERGY ELECTRONS BY ATMOSPHERIC GASES

V.Ye. Ivanov, N.K. Osipov and V.A. Shneyder

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The possibilities of using the kinetics of low energy electrons in the atmosphere are greatly limited both in certain methods [1-3] and in the Monte Carlo method [4] by the accuracy and form of the differential cross sections of their elastic scattering in atmospheric gases. Thus, when these cross sections are given in a form corresponding to the results of theoretical calculations and assuming their analytical integration over the scattering angle, in the Monte Carlo method there is a great reduction in the time necessary for achieving the given statistical accuracy. Taking this into account, we shall try to determine the analytical representations of differential scattering cross sections $I(E,\theta)$ of electrons with energies of E = 0.01-1 keV in the form of a polynomial in powers of the square of the change in the pulse of the scattered electron, corrected for the screening effect of the field of the electron shell nucleus. We shall limit ourselves to three terms, each of which prevails in the scattering region at small, average and large angles, respectively

$$I(E,\theta)=\sum_{i=1}^{3} A_i(E)\left\{\frac{2E}{R}[1-\cos\theta+2\eta]\right\}^{\alpha_i(E)}, \qquad (1)$$

where (2E/R) (1-cos θ) is the square of the change in the pulse of the scattered electrons; R — the constant equalling 13.6 eV;

* Numbers in margin indicate pagination in original foreign text.

θ — scattering angle; η — screening parameter; $A_1(E)$, $\alpha_1(E)$ — empirically selected coefficients depending only on energy.

When use is made of the VKB approximation, the expression for the screening parameter has the form

$$\eta = \eta_c \frac{1{,}7 \cdot 10^{-5} Z^{1/3}}{\tau(\tau+2)}, \quad \eta_c = 1{,}13 + 3{,}76\left[\frac{Z}{137v/c}\right]^2$$

where v— is the electron velocity; τ — electron kinetic energy in atomic units; Z — nucleus charge. However, according to calculations of [4] carried out for 1<E<20 keV and having a good agreement with the experimental data on electron energy dissipation [6,7], the value of the parameter η_c for the elastic scattering of low energy electrons (≤1 keV) may be assumed to be constant. Then

$$\eta = BE^{-1},$$

where B — is a constant; E — energy in units of eV. /243

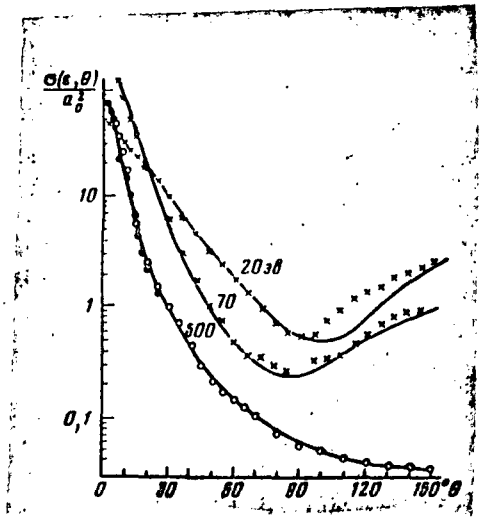

Figure 1.

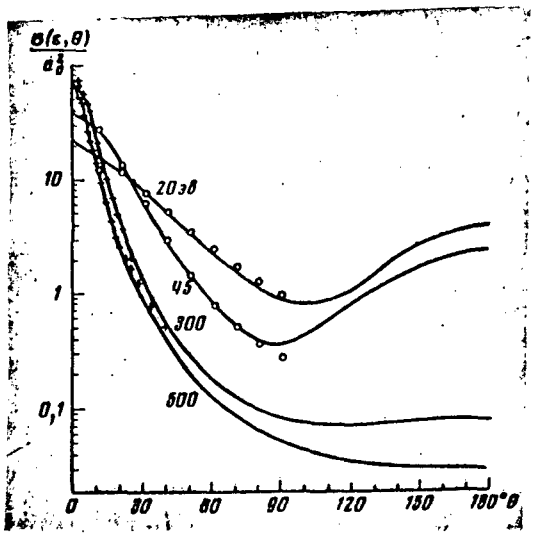

Figure 2.

Below we shall give the results of approximating the experimental data on scattering by nitrogen molecules [8] for electrons with E = 20 - 90 eV and the angular range of $3< \theta <160°$, data of [9] for E = 300,400, 500 eV and $2 \leq \theta \leq 40°$, and the data of [10] for the same energies and $4 \leq \theta \leq 150°$. At B = 2.38 the coefficients $A_1(E)$ and $\alpha_1(E)$ are approximated by the following expressions:

$$A_1(E) = 35 \cdot 10^{-\beta(E)}, \quad \beta(E) = \frac{1{,}98 \cdot 10^7 E^{-3{,}11}}{E^{0{,}028E} + 374}, \tag{2}$$

$$\alpha_1(E) = -\{1{,}04 \cdot 10^{12}[1 - 18{,}24(10/E)^5]^2 E^{-7{,}64} + 21E^{-0{,}61}\}, \tag{3}$$

$$A_2(E) = 301E^{-0{,}71} - 3{,}35 \cdot 10^5 E^{-2{,}2}, \tag{4}$$

$$\alpha_2(E) = -\{6{,}8E^{-0{,}29} - 10^3 E^{-2{,}71}\}, \tag{5}$$

$$A_3(E) = 8{,}39 \cdot 10^{-8}[1 + 1{,}5 \cdot 10^{-8} E^{3{,}2}]^{-1} E^{1{,}42}, \tag{6}$$

$$\alpha_3(E) = 53{,}4(1 - 2/E)E^{-0{,}64}. \tag{7}$$

Figure 1 gives examples of comparing the experimental data (dark circles — data from [9], light circles — data from [10], crosses — data from [8]) with the results of calculations using Formula (1) with the coefficients (2) - (7) (solid curves).

In a similar way, using data in [11, 12], we compiled the cross sections for scattering by molecular oxygen which, however, due to the absence of experimental data for large scattering angles was taken into account the same way as for N_2, i.e., the coefficients (6),(7). The validity of this approximation was controlled by comparing the integral scattering cross sections for O_2, calculated according to (1) with the measured integral cross sections. At B = 2.48 the coefficients $A_1(E)$ and $\alpha_1(E)$ of molecular oxygen have the following form:

$$A_1(E) = 11{,}15E^{0{,}193} \cdot 10^{-\beta(E)}, \quad \beta(E) = \frac{1{,}97 \cdot 10^7 E^{-3{,}03}}{E^{0{,}028E} + 374}, \tag{8}$$

$$\alpha_1(E) = -\{4{,}47E^{-0{,}15} + 6{,}73 \cdot 10^{10} E^{-7}\}, \tag{9}$$

$$A_2(E) = 310E^{-0{,}71} - 3{,}9 \cdot 10^3 E^{-1{,}86}, \tag{10}$$

$$\alpha_2(E) = -\{6{,}8E^{-0{,}29} - 943E^{-2{,}3}\}. \tag{11}$$

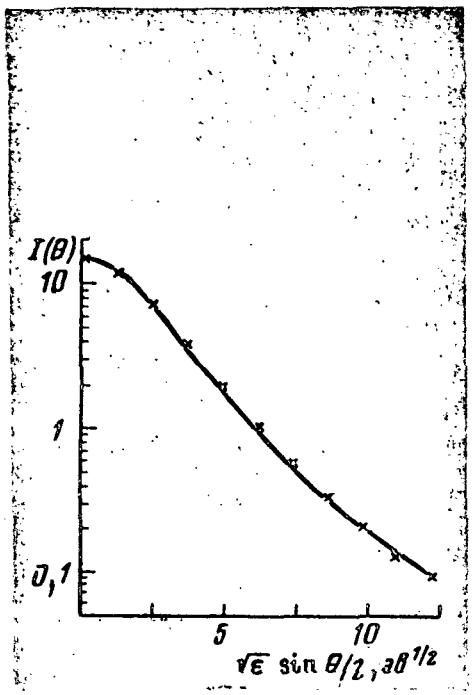

Figure 3.

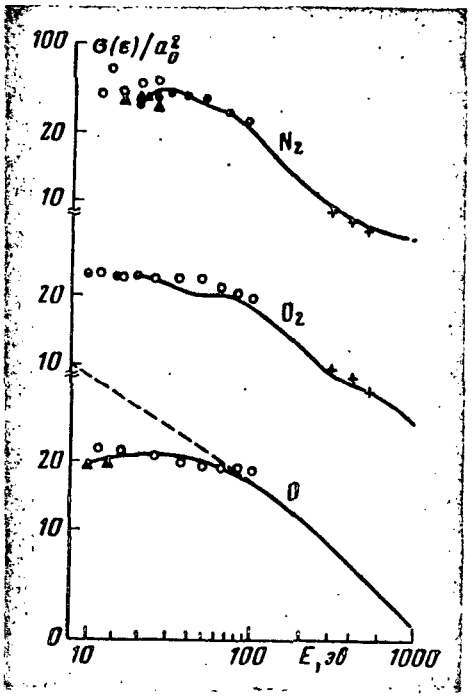

Figure 4.

Figure 2 shows experimental data on the cross sections of scattering by O_2 (crosses — data from [11], circles — [12]); these data were compared with the results of calculations using the approximations obtained.

There are no measurements of the differential cross sections for atomic oxygen. Therefore, when compiling their analytical expressions, we use the theoretical formulas obtained, introducing corrections in the field of small scattering angles. For this purpose, we standardized the integral cross sections calculated in the Bornov approximation to the measured integral cross sections. The initial material was the results of calculations in [13] carried out using the Hartree-Fokker method. The approximating expression for the scattering cross sections in this case has the form

$$I_1(E,\theta)=A_1\left[\frac{2E}{R}(1-\cos\theta+2\eta)\right]^{-2}+A_2\left[\frac{2E}{R}(1-\cos\theta+2\eta)\right]^{-\alpha}, \qquad (12)$$

where $A_1 = 182$, $A_2 = 5.28$, $B = 0.7$, $\alpha = 1.5$.

The degree of agreement between expression (12) and the Mott and Massy theory is illustrated in Figure 3, where the crosses designate the results of theoretical calculations. To correct the cross section given by Formula (12), we introduced the correction coefficient D(E), which decreases the scattering cross section by small angles in the low energy region

$$I(E,\theta)=D(E)A_1\left[\frac{2E}{R}(1-\cos\theta+2\eta)\right]^{-2}+A_2\left[\frac{2E}{R}(1-\cos\theta+2\eta)\right]^{-\alpha}. \qquad (13)$$

The correction coefficient D(E) is found from the conditions for standardizing the integral elastic scattering cross sections calculated from (12) to the total scattering cross sections measured in [14]: /245

$$D(E)=\frac{\sigma_p(E)-2\pi A_2\int_0^{\pi}[(2E/R)(1-\cos\theta+2\eta)]^{-\alpha}\sin\theta\,d\theta}{2\pi A_1\int_0^{\pi}[(2E/R)(1-\cos\theta+2\eta)]^{-2}\sin\theta\,d\theta}, \qquad (14)$$

where $\sigma_p(E)$ is the experimentally measured total scattering cross section of electrons by atomic oxygen. The approximating expression given below is obtained for the correction D(E) calculated according to (14):

$$D(E)=1-\exp(-0{,}02E).$$

Let us compare the integral elastic scattering cross sections calculated for N_2 and O_2 using (1) and for O using (13), with the experimental measurements of the latter. Figure 4 compares the integral cross sections for N_2 calculated by integrating Formula (1) (solid line) with the total cross sections measured in [15] (light circles), [16] (triangles), and with the integral cross sections obtained by numerical integration of experimental data [8]

(solid circles) and [9] (crosses). Figure 4 performs a similar comparison for molecular oxygen with measurements of [14] (light circles), [17] (dark circles) and [11] (crosses). In addition, it also gives similar data for atomic oxygen (calculated according to (13) — solid lines, circles — [14], theoretical calculations given in [13] — triangles; the dashed curve corresponds to the integral cross section calculated according to (12)). Figure 4 gives the results of comparing the experimental data with the calculations. These data show that the approximations obtained represent reliable material which can be used in calculations of electron transfer.

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